OPTIMIZATION OF VARIANCE REDUCTION PARAMETERS IN MONTE CARLO RADIATION TRANSPORT CALCULATIONS TO A NUMBER OF RESPONSES OF INTEREST

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ABSTRACT

Radiation transport problems involving high attenuation require non–analogue Monte Carlo techniques which conserve the first moment whilst reducing the variance and are normally directed at a single response. Variance reduction parameters appropriate to one response may not necessarily be appropriate to another. This paper outlines an approach to the problem of variance reduction optimization to several responses simultaneously. The technique is based on the DSA (Direct Statistical Approach).

I. INTRODUCTION

In radiation transport calculations, analogue Monte Carlo (i.e. simulation) is employed when the required flux or response may be estimated to a reasonable statistical error with an acceptable computing time. When this becomes too time–consuming, variance reduction methods must be employed which conserve the first moment whilst reducing the second moment and variance. As they employ in some form an estimate of the adjoint flux which is strictly linked to a single response, such methods are normally directed at one response: a flux or some function of the flux. The variance reduction parameters ("vr parameters") appropriate to one response (in that they reduce the statistical error) may not be appropriate to another. Thus Monte Carlo may treat problems involving a high attenuation only by calculating a single response at a time.

The technique proposed here to calculate several responses simultaneously with non–analogue Monte Carlo is based on the DSA (Direct Statistical Approach, Refs. 1, 2 and 3). The DSA optimises vr parameters controlling the track population (Ref. 2) or weight (Ref. 3) in fixed source problems currently involving neutron and photon transport. It employs the code MCNP (Ref. 4) as a vehicle. The objective is to generate vr parameters that attempt to both equalise and minimize the fractional standard deviations (fsd's) attached to the various responses (see Sec. II).

II. THEORETICAL BACKGROUND

The DSA expresses the second moment, S^2, and the time τ, per source history, in terms of the unknown vr parameters [either phase space cell importances for population control (Ref. 2) or phase space cell starting weights for weight control (Ref. 3)] and problem–dependent coefficients [involving transfer probabilities and accumulated weights between cell boundaries (and between the source and cell boundaries, and cell boundaries and the detector)] that are to be estimated. For population control, under normal conditions, both S^2 and τ are separable. For weight control an approximation must be made to render S^2 separable (Ref. 3). Once separable, standard minimization routines are used to find the set of parameters that renders q minimum, where:

$$q \quad = \quad S^2 \; . \; \tau \tag{1}$$

q^{-1} is a reasonable measure of the efficiency of a Monte Carlo calculation (Ref. 5). We write expression (1) for response i as:

$$q_i \quad = \quad S_i^2 \; . \; \tau \tag{2}$$

We now normalize the second moments using the squares of the respective first moments, D_i and sum over M responses, employing the subscript "fc" standing for "fractional and compound":

$$q_{fc} = \sum_{i=1}^{M} \frac{q_i}{D_i^2} = \sum_{i=1}^{M} \frac{S_i^2}{D_i^2} \cdot \tau \tag{3}$$

The "figure of merit" (fom) used as a measure of the quality of a calculation in codes such as MCNP is defined as:

$$\text{fom} = (\text{fsd}^2 \cdot T_S)^{-1} \tag{4}$$

where fsd is as before and T_S is the computing time for a sample of N independent histories. Defining a "compound fom" (fom_c) for M responses as:

$$\text{fom}_c = \left(\sum_{i=1}^{M} (\text{fsd}_i)^2 \cdot T_S \right)^{-1} \tag{5}$$

then $(q_{fc})^{-1}$ is equal to fom_c assuming that D_i^2 is much less than S_i^2. Thus our objective is to maximize fom_c by estimating S_i^2 and τ (and D_i). The form of S^2 and τ are found in Refs. 2 and 3.

III. DEMONSTRATION PROBLEM

Under study is the conversion of the TAPIRO reactor (Ref. 6) at ENEA Casaccia, Italy to a boron neutron capture therapy (BNCT) facility. TAPIRO is a fast assembly with core radius 6.3 cm and height 10.87 cm with 93.5% enriched uranium metal and a copper reflector. A sector of the concrete shield and outer reflector has been replaced by a structure whose role is to provide an epithermal neutron spectrum. That considered here, suggested by Rief *et al.* (Ref. 7), is a sequence of five modules, each consisting of 2 cm of D_2O and 8 cm of aluminium, followed by 11.5 cm of aluminium, 0.4 mm of cadmium and 13 cm of lead. The "spectrum shifter" is surrounded by a nickel reflector. Following the lead, there is a graphite collimator which restricts the neutron beam to a 10 cm radius aperture (see Fig. 1). It is emphasised that the configuration employed in this test problem is not the final one.

BNCT is appropriate for a multi–response optimization as the neutron spectrum is required over the whole energy range as well as the gamma ray dose. One seeks to maximize the epithermal flux whilst minimizing the thermal and fast components and the gamma dose.

The DSA Cell Importance model (Ref. 2) with 140 phase space cells (28 spatial, 5 energy) was employed to control the track population. The first objective was to calculate the neutron spectrum at the collimator exit. Figs. 2, 3 and 4 show this spectrum from a 30 min calculation (IBM RISC 6000, Model 43P, op. sys. AIX), employing one, three and five responses of interest respectively (cases "a", "b" and "c"). [The responses being the flux over the whole energy range (i.e. the total flux), the thermal (< 1 eV), epithermal (1 eV – 10 keV) and fast (> 10 keV) fluxes, and the lower thermal (< 0.32 eV), upper thermal (0.32 – 1 eV), epithermal (1 eV – 10 keV), lower fast (10 keV – 1 MeV) and upper fast (> 1 MeV) fluxes.] (The flux units were: n cm^{-2} sec^{-1}.) In Figs. 2 – 4 we see an increase in the statistical quality over the whole energy range as the number of responses increases. This is the main result of this paper.

The time required to generate the optimum vr parameters increases with the number of responses. Whilst an objective measure of this time is not available, case "b" took about twice the time of case "a" and case "c" took just under five times the time. As the number of responses increases, time lost to internal book–keeping becomes appreciable. It is hoped in the future to reduce this.

It was also of interest to attempt to calculate the gamma ray dose at the collimator exit at the same time as the neutron spectrum. In this neutron–gamma calculation, a further 5 energy groups were used for the gammas, making a total of 280 phase space cells. Optimum vr parameters were generated for the three neutron responses (thermal, epithermal and fast flux) and the gamma dose (case "d"). Running with these parameters gave results for the neutron spectrum that were of slightly poorer quality (a factor of 1.2 to 1.6) compared with case "b" above as time is being lost in simultaneously tracking the gammas. Results after 56 min CPU time were as follows:

optimization to 3 neutron fluxes plus the gamma dose (case "d"):	result	fsd
Φ_n: < 1 eV (n cm^{-2} sec^{-1}):	$1.41 . 10^8$	.0348
Φ_n: 1 eV – 10 keV (n cm^{-2} sec^{-1}):	$5.44 . 10^8$	.0287
Φ_n: > 10 keV (n cm^{-2} sec^{-1}):	$2.65 . 10^7$	.0369
gamma ray dose equivalent (μSv/hr):	$2.71 . 10^5$	.0833

We see that the error on the gamma dose is appreciably higher than that on the neutron fluxes. Most of this dose comes from gammas born from neutron absorption in the concrete to the left of the collimator in Fig. 1. Neutrons producing these gammas have already passed through the collimator and contributed to the neutron flux. Thus the optimum in this problem must involve lower statistical errors on the neutron responses compared to the gamma response.

In cases "b" and "d", a verification was made of the possible saving in computer time employing the simultaneous optimization to M responses compared with M separate single–response optimizations. To achieve a given fsd on each response, one calculation with the set of vr parameters optimized to M responses simultaneously gave a 37% saving (case "b") and a 43% saving (case "d") compared with M calculations with the sets of vr parameters optimized to each response. Concerning the time to generate the vr parameters, again with the proviso of lack of objectivity, similar times were noted for both cases. The main saving is in human time. Each optimization consists of a series of iterative steps (see Ref. 3) and the multi–response optimization needs to go through this procedure once only.

Finally the single–response DSA was compared with standard importance–based methods. A weight window produced by MCNP's weight window generator (Ref. 4) gave results that were a factor of around 2.5 poorer than those of the DSA for the total neutron flux at the collimator exit and a factor of around 5 poorer for the gamma dose.

IV. CONCLUDING REMARKS

The results of this first attempt at multi–response optimization in Monte Carlo with the DSA are promising. As the number of responses increases, the CPU time lost to internal book–keeping becomes considerable. Future efforts will concentrate on reducing this. The responses considered were at the same spatial location. The responses may also be located at different positions although the optimal calculation with certain combinations of locations might not give an advantage over keeping the calculations separate.

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Fig. 1: TAPIRO; geometry; horizontal section

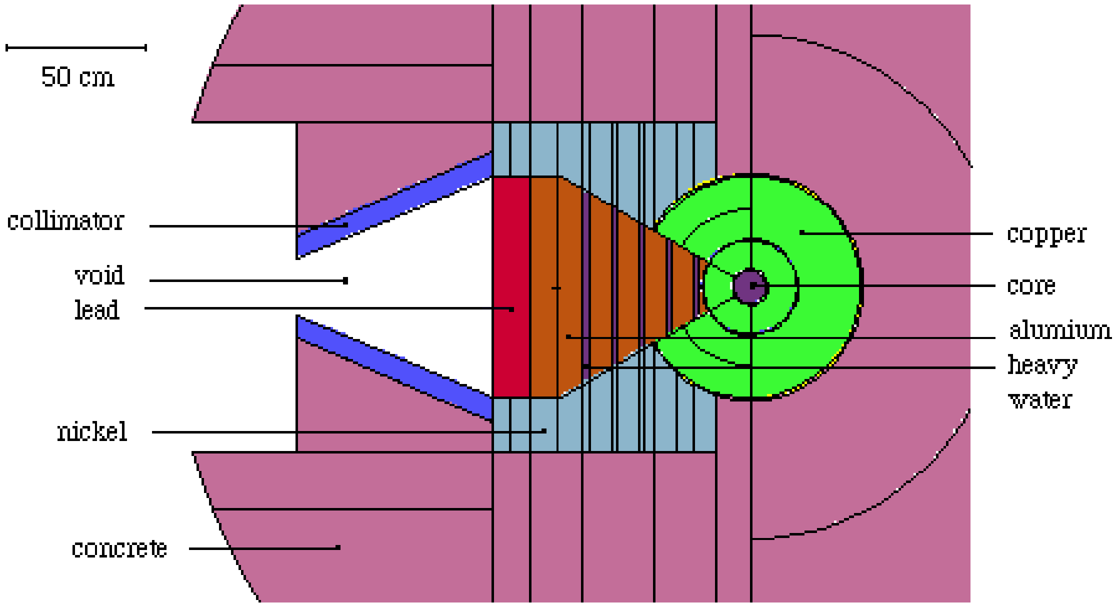

Fig. 2: TAPIRO; 1 neutron group; 30 min (case "a")

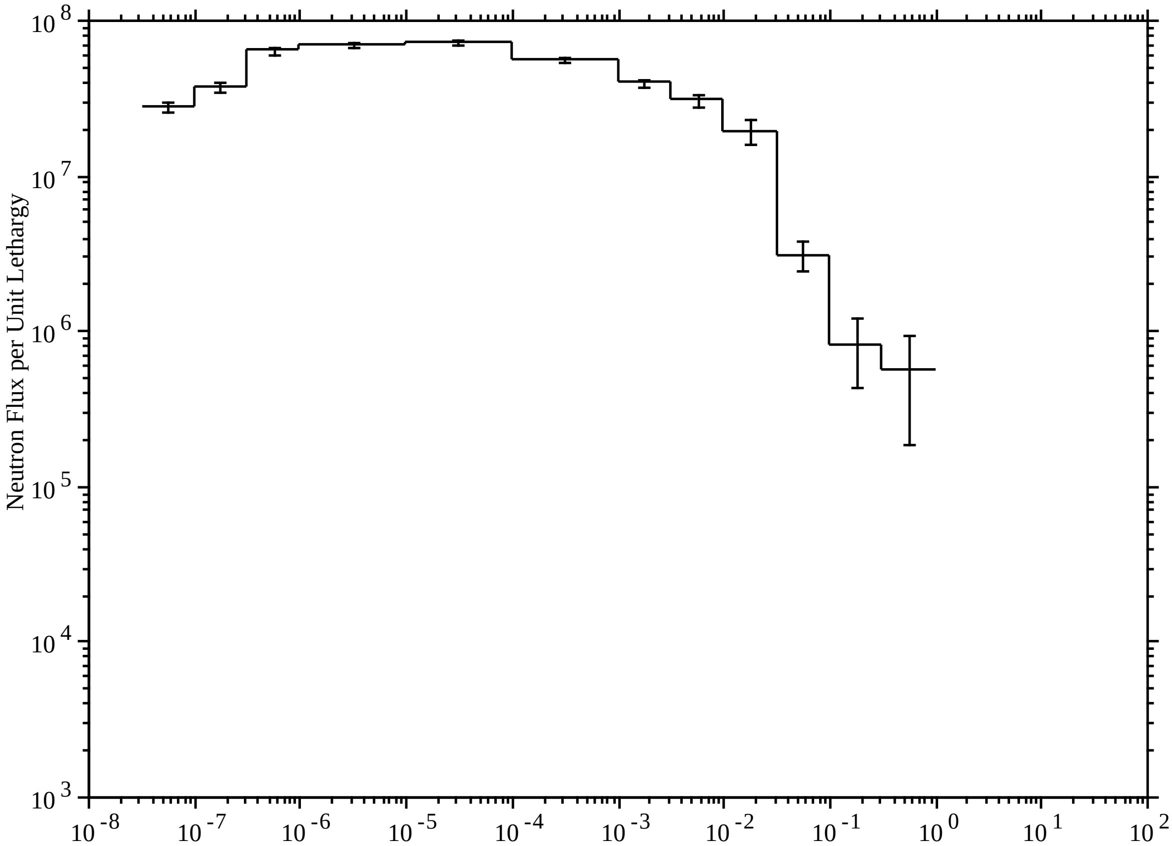

Fig. 3: TAPIRO; 3 neutron groups; 30 min (case "b")

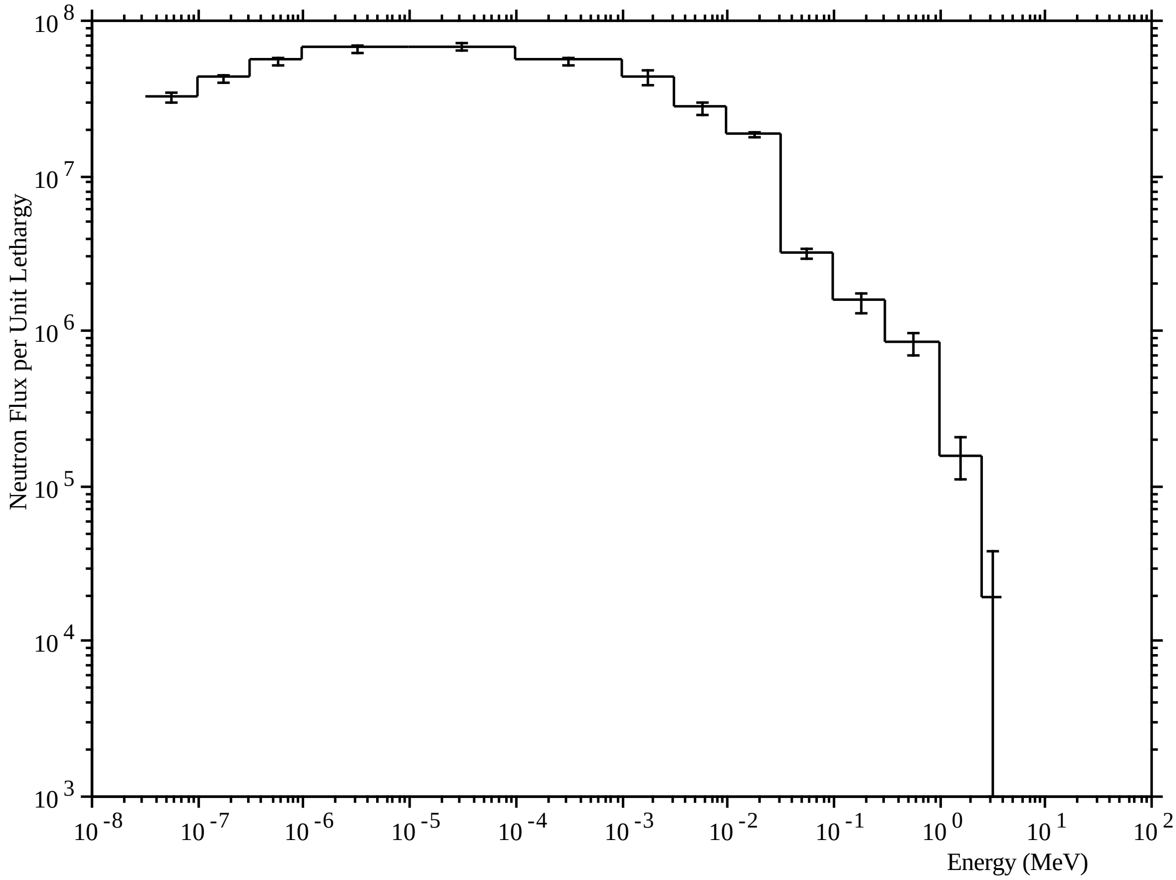

Fig. 4: TAPIRO; 5 neutron groups; 30 min (case "c")